Finally Summary for NCC 2903
Molecular Modeling of Polymer Electrolytes

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We performed high-level ab initio electronic structure calculations on complexes of the model ethers dimethylether, 1,2-dimethoxyethane, and 1,2-dimethoxypropane with Li^+ cations and Cl^- and I^- anions. Based upon these studies, an accurate intermolecular potential for these systems, including a two-body representation of polarization effects, was developed. This work is published as "Quantum Chemistry Study of the Interactions of Li^+, Cl^- and I^- Ions with Model Ethers", G.D. Smith, R.L. Jaffe and H. Partridge, *J. Phys. Chem. A* **1997**, 101, 1705. Using the quantum chemistry-based potential, we performed molecular dynamics simulations of poly(ethylene oxide) with LiI. We studied the cation environment, mobility, the system conductivity, and polymer conformations as a function of temperature, salt concentration, and chain crosslinking. This work is published as "Polymer force fields from ab initio studies of small model molecules: can we achieve chemical accuracy?," G.D. Smith et al., *Spectrochimica Acta A* **1997**, 53, 1273 and "The Cation Environment in Molten LiI Doped Poly(ethylene oxide)," J.D. Londono et al. *Macromolecules* in press. This work was also presented at the Spring 1996 meeting of the American Physical Society in Kansas City, Mo.

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